Comment on "First-principles calculation of the superconducting transition in MgB_2 within the anisotropic Eliashberg formalism"

I. I. Mazin[1], O. K. Andersen[2], O. Jepsen[2], A. A. Golubov[3], O. V. Dolgov[2,4], and J. Kortus[2]
[1] *Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375-5000, USA*
[2] *Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany*
[3] *University of Twente, Department of Applied Physics, 7500 AE Enschede, The Netherlands*
[4] *Eberhard-Karls-Universität, Auf der Morgenstelle 14, D-72076 Tübingen, Germany*
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In a recent paper[1], as well as in a follow-up paper[2], Choi et al. reported a novel computational implementation of ideas proposed in Ref. 3 and implemented in the form of a two-gap model in Refs. 4,5. Choi et al.'s treatment of the fully anisotropic Eliashberg equations differs from the early treatment[6] of the isotropic Eliashberg equations by integrating out all phononic- rather than all electronic degrees of freedom, and is a timely and most valuable contribution to the theory of superconductivity in MgB_2. However, because of Choi et al.'s strong claim that their results can be compared directly with the experiment, a few comments seem to be in place.

1. Ref. 1 implies that there is a distribution of gaps *within* the σ and the π-sheets, not only in the calculations for perfectly clean MgB_2, but also in the actual material; in other words, that the distribution of gaps shown in Fig. 2 of Ref. 2 is *observable.* However, in the theory of anisotropic superconductivity it is known that any intraband nonuniformity of the order parameter is suppressed by intraband impurity scattering. The dimensionless parameter that controls this suppression is (see, *e.g.*, Ref. 7) $\alpha = (\delta\Delta/\bar{\Delta})^2(kT_c/\gamma)$, where $\delta\Delta$ and $\bar{\Delta}$ are, respectively, the rms variation and the average value of the order parameter, T_c is the critical temperature, and γ is the impurity scattering rate. If $\alpha \ll 1$, the variation is smeared out. For the σ and π-bands, respectively, this parameter is only $(0.5\,\mathrm{meV}/7\,\mathrm{meV})^2(3.5\ \mathrm{meV}/\gamma) \sim 0.02\,\mathrm{meV}/\gamma$ and $(0.5\,\mathrm{meV}/2\,\mathrm{meV})^2(3.5\ \mathrm{meV}/\gamma) \sim 0.2\,\mathrm{meV}/\gamma$. Obviously, any perceivable sample of MgB_2 has $\gamma \gg 0.2$ meV, so that $\alpha \ll 1$ for both bands. It is worth mentioning that even the fact that the 5 meV gap difference between the σ and the π-bands is not smeared out is surprising, and seems to be due to the the inability of common impurities to couple between the disparate σ and π-band wavefunctions[8], so that $\gamma_{\sigma\pi} \ll \gamma_{\sigma\sigma} \sim \gamma_{\pi\pi}$. Therefore, in any foreseeable experiment at most two distinct gaps may be observed.

2. The anisotropic Eliashberg equations 1 of Ref. 1 contain the factor $\lambda(\mathbf{k},\mathbf{k}',\nu-\nu') - \mu^*(\omega_c)$. For the Coulomb pseudopotential, Choi *et al.* used $\mu^*(\omega_c) = 0.12$ (with the cut-off frequency $\omega_c \approx 5\omega_{ph}^{\max}$) and claimed to have shown that the superconducting properties of MgB_2 are not very sensitive to the choice of $\mu^*(\omega_c)$. Below, we shall argue that taking $\mu^*(\omega_c)$ to be independent of $\mathbf{k}$ and $\mathbf{k}'$ is hardly a realistic approximation and may be a misstatement of the calculations reported in Refs. 1,2. In fact, due to the very small overlap of the σ- and π-band charge densities, the $\sigma\pi$-interband Coulomb matrix elements are considerably smaller than the intraband matrix elements[4], and taking this into account influences the superconducting properties more than the difference between the two-gap treatment and the fully anisotropic treatment

This we shall now demonstrate. Choi *et al.* do not give the band-integrated values of their coupling constants, but by integrating Fig. 3 of Ref. 1 with the DOS-ratio $N_\pi/N_\sigma = 1.37$ according to:

$$\lambda_{nn'}(0) \equiv \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'}\frac{\delta(\varepsilon_{n\mathbf{k}})}{N_n}\lambda(\mathbf{k},\mathbf{k}',0)\delta(\varepsilon_{n'\mathbf{k}'}) \qquad (1)$$
$$= \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'} W_{n\mathbf{k}}\,\lambda(\mathbf{k},\mathbf{k}',0)W_{n'\mathbf{k}'}N_{n'}$$

for the phonon-mediated coupling of an electron in band n to all electrons in band n', we can map Choi *et al.*'s fully anisotropic model onto a two-gap model with $\lambda_{\sigma\sigma} = 0.78$, $\lambda_{\sigma\pi} = 0.15$, $\lambda_{\pi\sigma} = 0.11$, and $\lambda_{\pi\pi} = 0.21$. These λ-values yield the mass-renormalization parameters in Fig. 2 of Ref. 1: $m^*/m - 1 = \lambda_\sigma = \lambda_{\sigma\pi} + \lambda_{\sigma\sigma} \approx 0.94$ and $\lambda_\pi = \lambda_{\pi\sigma} + \lambda_{\pi\pi} \approx 0.32$. The total isotropic (thermodynamic) $\lambda = (N_\sigma\lambda_\sigma + N_\pi\lambda_\pi)/N = 0.61$, which of course is the same as the one given by Choi *et al.*. Here, and in Eq. 1, N is the DOS summed over all bands. With this two-gap model we have performed strong-coupling Eliashberg calculations in order to compare the results for T_c and the gaps with those resulting from the fully anisotropic treatment. For all four spectral functions we used the isotropic $\alpha^2F(\omega)$ from Fig. 1 of Ref. 2 scaled to produce the λ-matrix given above. The $\mu^*(\omega_c)$-matrix is obtained from Eq. 1 with $\lambda(\mathbf{k},\mathbf{k}',0)$ substituted by Choi *et al.*'s $\mu^*(\omega_c)$. The resulting T_c and the gaps are shown by dashed lines in Fig. 1 as functions of $\mu^*(\omega_c)$. At $\mu^*(\omega_c) = 0.12$, as used by Choi *et al.*, we get $T_c = 43$K, $\Delta_\sigma = 7.2$ meV, and $\Delta_\pi = 1.3$ meV. The corresponding values quoted by Choi *et al.* are 39K, 6.8 meV and 1.8 meV. These differences are hardly due to intraband anisotropy, first of all because it can only increase T_c. Secondly, increasing the number of gaps from two to four in the Eliashberg equations, which should catch most of the anisotropy beyond the two gap model, we found rather small changes[9].

If, however, we assume that Choi *et al.* used $\mu^*(\omega_c)\delta_{nn'}$, *i.e.* that they had no Coulomb repulsion between the σ and π-electrons, then the corresponding two-

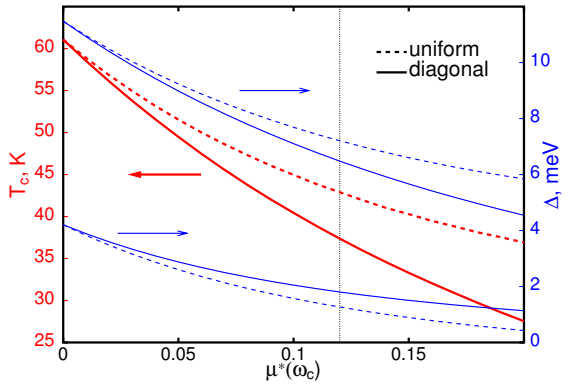

FIG. 1: Critical temperature and the values of the σ and π gaps at 1 K as function of the renormalized Coulomb pseudopotential, $\mu^*(\omega_c)$, in two models: The uniform model where all matrix elements of the Coulomb repulsion are equal and the diagonal model where the interband matrix elements are zero. In both cases the normalization is chosen so as to produce given values of $\mu^*(\omega_c)$ after proper summation over all bands.

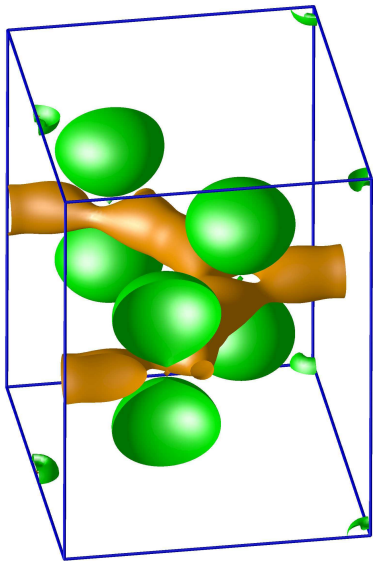

FIG. 2: Constant-density contour for the normalized σ (orange) and π (green) electron-densities, $|\psi(\mathbf{r})|^2_\sigma$ and $|\psi(\mathbf{r})|^2_\pi$, at the Fermi level.

gap treatment gives the full lines in Fig. 1 and, hence, $T_c = 38K$, $\Delta_\sigma = 6.5$, and $\Delta_\pi = 1.8$ for $\mu^*(\omega_c) = 0.12$, in nearly perfect agreement with the numbers quoted by Choi *et al.* (perfect agreement can be attained with $\lambda_{\sigma\sigma} = 0.80$ and $\lambda_{\pi\pi} = 0.20$). It seems likely that the algorithm actually encoded by these authors fully neglects the off-diagonal Coulomb repulsion, as opposed to using a uniform repulsion, as suggested by their Eq. 1.

That uniform and diagonal Coulomb pseudopotentials yield quite different results is not surprising: the same total Eliashberg μ^* in the uniform case is distributed over intra- and interband terms so that the $\sigma\sigma$-part of the pairing interaction suffers less than in the case of a diagonal μ^*, and the $\sigma\pi$-part suffers more. $\lambda_{\sigma\sigma}$ is more important for the critical temperature, and $\lambda_{\sigma\pi}$ for generating Δ_π. For uniform μ^*, therefore, the T_c and Δ_σ are larger, and Δ_π is smaller.

Having demonstrated that the assumed structure of μ^* matters[10] for the superconducting properties of MgB_2, let us estimate this structure from first principles. The unrenormalized μ is the total density of states times the matrix element $\langle n\mathbf{k}\uparrow, n-\mathbf{k}\downarrow|V_C|n'\mathbf{k}'\uparrow, n'-\mathbf{k}'\downarrow\rangle$ for scattering a Cooper pair from state $|n'\mathbf{k}'\rangle$ to state $|n\mathbf{k}\rangle$ via a phonon of wave-vector $\mathbf{k}-\mathbf{k}'$. Inserting this in Eq. 1 instead of $\lambda(\mathbf{k},\mathbf{k}',0)$ yields $\mu_{nn'}$. Here $V_C(\mathbf{r},\mathbf{r}')$ is the screened Coulomb interaction between the electrons, and since it has short range in good metals, it makes sense to take it proportional to the delta-function $V_C\delta(\mathbf{r}-\mathbf{r}')$. This leads to the following estimate:

$$\mu \sim V_C N \int |\psi_{n\mathbf{k}}(\mathbf{r})|^2 \, |\psi_{n'\mathbf{k}'}(\mathbf{r})|^2 \, d^3r$$
$$\mu_{nn'} \sim V_C N_{n'} \int |\psi(\mathbf{r})|^2_n \, |\psi(\mathbf{r})|^2_{n'} \, d^3r, \qquad (2)$$

where $|\psi(\mathbf{r})|^2_n \equiv \sum_{\mathbf{k}} |\psi_{n\mathbf{k}}(\mathbf{r})|^2 \, \delta(\varepsilon_{n\mathbf{k}})/N_n$ is the shape, normalized to 1 in the cell or the crystal, of the electron density of band n at the Fermi level. These σ and π densities are shown in Fig.2, and they yield for the ratios of the integrals in Eq.2

$$\left\langle |\psi|^4_\sigma \right\rangle : \left\langle |\psi|^4_\pi \right\rangle : \left\langle |\psi|^2_\sigma \, |\psi|^2_\pi \right\rangle \sim 3.0 : 1.8 : 1. \qquad (3)$$

These ratios reflect the facts that the σ-density is more compact than the π-density, and that the overlap of these two densities is small. Note that the exceptional smallness of the interband impurity scattering[8] in MgB_2 is due not only to this difference in charge density, but also to a disparity of the σ and π *wave functions*.

From Eqs. 2, 3 we get: $\mu_{\sigma\sigma} : \mu_{\pi\pi} : \mu_{\sigma\pi} = 2.2 : 1.8 : 1$. Now, any anisotropy in the *bare* pseudopotential is further *enhanced* in the renormalized μ^* : in the one-band case μ is renormalized as $\mu^*(\omega_c) = [1 + \mu \ln(W/\omega_c)]^{-1} \mu$, where W is a characteristic electronic energy of the order of the bandwidth or plasma frequency. For the multiband case, this is a matrix equation with W being a diagonal matrix with elements W_n. Assuming for simplicity that $\mu_{\sigma\sigma} = \mu_{\pi\pi} = A\mu_{\sigma\pi}$ with $A > 1$, and that $\mu_{\sigma\sigma} \log(W_\sigma/\omega_c) = \mu_{\pi\pi} \log(W_\pi/\omega_c) = L$, one obtains: $A^* = A + (A - A^{-1})L$. For MgB_2, $L \sim 0.5 - 1$ and $A \sim 2.3$, so that $A^* \sim 3 - 4$, which is very different from the uniform μ.

In conclusion: Although of academic interest, any difference between the results of the fully anisotropic Eliashberg formalism and those of the two-gap formalism will hardly be observable in real MgB_2-samples. On the other hand, the $(\mathbf{k},\mathbf{k}')$-, or rather (n,n')-dependence of the Coulomb pseudopotential does have an observable effect on the calculated critical temperature and the gap ratio.

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[9] This is not surprising, given that the variation of the calculated order parameter[2], as well as of the mass renormalization[1], within each band is at most 10%.

[10] The problem of proper structure of the μ^*-matrix is specific for multiband superconductivity with large gap disparity. When the pairing interaction is fully uniform, the μ^* matrix can have any structure as long as it is normalized to the total μ^*. This has no effect on either T_c or gap-ratios.